2,2,8-Trimethyl-7-prop-2-ynoxychromene 94244-29-8 | DTXSID10241225

94244-29-8	D1X5ID10241225	

Model Performance

Model	Data

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 4.29e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.71e-01

Confidence level: 5.94e-01

Nearest Neighbors from the Training Set

Image not found

2-Ethylanthracene Measured: 1.05e-04 Predicted: 6.24e-06

Image not found

Fluazuron

Measured: 7.57e-05 Predicted: 1.00e-09

Image not found

Isazofos

Measured: 7.19e-06 Predicted: 4.87e-05

Image not found

Diphenylurea

Measured: 1.50e-04 Predicted: 1.72e-06

Image not found

2,4,5-Trichlorophenoxyacetic

acid

Measured: 1.50e-05 **Predicted:** 4.08e-06